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Origins of interfacial disorder in GaSb/InAs superlattices

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The interface surfaces of short-period GaSb/InAs superlattices grown by molecular beam epitaxy have been studied *in situ* with scanning tunneling microscopy. Migration enhanced epitaxy was used at the interfaces in order to control bond type. Interfaces on GaSb(001) are found to be smoother than those on strained InAs(001), and the InSb-like interfaces are smoother than GaAs-like ones. The primary source of disorder at these interfaces appears to be the kinetically determined topography of the growth surfaces, with intermixing playing a secondary role. © 1995 American Institute of Physics.

The strained-layer, type-II $Ga_{1-x}In_xSb/InAs$ superlattice system is a promising alternative to the $Hg_{1-x}Cd_xTe$ system for use in infrared detectors. With a widely tunable band gap, comparable absorption coefficients, and potentially greater sensitivity, the superlattice system has the additional advantage that it can be fabricated using reproducible III–V semiconductor molecular beam epitaxy (MBE) methods. Unfortunately, currently achieved electronic mobilities in short-period superlattices are much less than those theoretically predicted, a shortfall attributed to interfacial disorder. 4

It is useful to distinguish between two possible sources of interfacial disorder: roughness and intermixing. Roughness is defined as variations in the topography at an interface. These variations include monolayer-height (~3 Å) steps resulting from any misorientation of the starting wafer and, more significantly, multiple layers of islands and pits (vacancy islands) caused by kinetic and/or thermodynamic effects during growth. There may also be growth-related roughness on the atomic scale (~0.3 Å) associated with local variations in the surface lattice. In contrast, disorder due to intermixing occurs when diffusion, exchange reactions, etc. take place between different elements at an interface. The extent of this disorder is determined by the thermodynamics of the interface and the kinetics of the reactions.

The disorder at GaSb/InAs interfaces has been recently characterized with a variety of techniques, including crosssectional scanning tunneling microscopy (XSTM), 5,6 crosssectional high-resolution transmission electron microscopy (XHRTEM), Raman spectroscopy, and x-ray diffraction. Either InSb-like or GaAs-like interfaces can be grown on either GaSb or InAs surfaces; ⁹ XSTM studies found that both the GaAs-like and InSb-like interfaces have a similar degree of disorder,⁵ but that interfaces grown on InAs are generally more ordered than those grown on GaSb. 5,6 These studies concluded that intermixing is the primary source of disorder.^{5,6} In contrast, recent XHRTEM images have shown that GaAs-like interfaces are significantly more disordered than InSb-like interfaces. When considered in conjunction with Raman and x-ray results, 8 these images led Twigg et al. to conclude that roughness, not intermixing, is the major source of disorder.⁷ To directly address the origins of interfacial disorder in these superlattices, we have used STM to study the surfaces of short-period GaSb/InAs superlattices *in situ* as a function of interface.

Our experiments were carried out in an interconnected, multichamber ultrahigh vacuum (UHV) facility that includes a III–V semiconductor MBE chamber and a surface analysis chamber with STM. After thermally removing the oxide from each GaSb(001) substrate, a 1 μ m-thick buffer layer of GaSb was grown at 470 °C, and then cooled to 400 °C under an Sb flux. GaSb/InAs superlattices were then grown at 400 °C, the optimal growth temperature, with an InAs growth rate of 0.2 monolayers (ML)/s and a GaSb growth rate of 0.5 ML/s. 8.9

Although the epilayers were generally grown using III–V codeposition, migration enhanced epitaxy (MEE) was used at each interface in order to optimize interface abruptness. ^{8,9} For example, to form the InSb interface on GaSb, the Ga shutter was closed and the Sb flux allowed to continue for 5 s. A monolayer of In was then deposited while there was no anion flux. To continue the superlattice, In and As were then codeposited to grow InAs. For interfaces to be examined by STM, the cation monolayer was terminated by an appropriate anion soak (arsenic for the example above), and then cooled to room temperature in the absence of any flux.

An image of the surface of a typical GaSb buffer layer is shown in Fig. 1(a). The surface consists of large, atomically smooth terraces (~500 Å wide) separated by monolayerheight (3.0 Å) steps, with very few islands or pits. (The pits result from island coalescence.) This surface appears to be close to thermodynamic equilibrium, so that the average terrace width is determined by the misorientation of the sample with respect to (001). Atomically resolved images of each terrace (not shown) reveal the Sb-terminated 1×3 surface reconstruction, 11 consistent with reflection high-energy electron diffraction (RHEED). The stability of the $[1\overline{1}0]$ -oriented rows of Sb dimers inherent to this reconstruction gives the terrace edges their characteristically straight [110]-oriented and jagged [110]-oriented edges. 12 Thin GaSb films (8 ML) grown at 400 °C within the superlattice have a very similar surface structure (atomically smooth terraces with few islands and pits), but with more rounded terrace edges.

Our characterization of the GaSb/InAs interfaces will fo-

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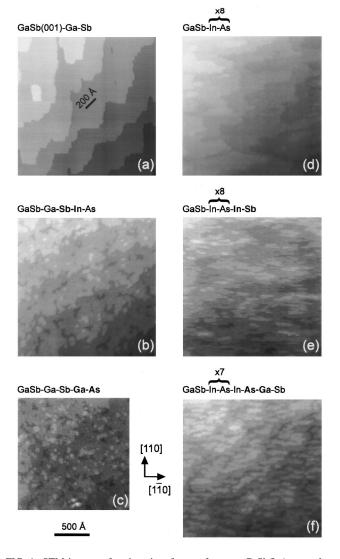


FIG. 1. STM images of various interface surfaces on GaSb/InAs superlattices. The images were acquired with a constant current of 0.1 nA and sample biases between -1.8 and -2.2 V. (a) GaSb(001) buffer layer; (b) InSb-like interface on GaSb; (c) GaAs-like interface on GaSb; (d) eight monolayer-thick strained InAs(001) epilayer on GaSb; (e) InSb-like interface on InAs; (f) GaAs-like interface on InAs. The top-most atomic layers at each surface are indicated, with the nominal interface bond type in bold. An (001) plane has been subtracted from each image so that each terrace level appears approximately as a single gray level. Note that all the images are displayed at the same lateral scale.

cus on the disorder due to roughness, defined as the number of additional monolayers present on each terrace at the completion of interface growth. It can be characterized on any length scale, but we will focus on two here: (1) the total roughness on each terrace, a good indication of the overall roughness associated with the growth; and (2) the roughness within a typical 200 Å-long line oriented in the $\langle 100 \rangle$ direction, a sampling comparable to that viewed by XHRTEM. The roughness on the clean GaSb(001) surfaces, as defined here, is approximately 0 ML on both length scales.

The addition of an interface layer to a $GaSb(001)1\times 3$ surface causes significant changes to the surface morphology. Following the growth of an As-terminated InSb interface [Fig. 1(b)], small 1 ML-deep pits and 1 ML-high islands

(\sim 100 Å-diameter) are now observed on each terrace, giving the terraces a roughness of 2 ML. Due to the low density of these features, the typical roughness on the XHRTEM length scale (200 Å) is only 1 ML (i.e., along this length either a pit or an island would typically be encountered). The islands and pits, the more rounded and meandering shape of the terrace edges, and the additional roughness observed on the atomic scale are all indications that the surface has not reached its equilibrium structure. Following deposition of the GaAs interface on GaSb(001) [Fig. 1(c)], even more extensive roughening is observed. Small pits and islands are now observed on each terrace, as on the InSb-like interface, but with approximately equal areas and twice the density. This surface has a terrace roughness of 2 ML and a "200 Å" roughness of 2 ML; the GaAs surface is also noticeably rougher on the atomic scale than the InSb interface.

The InAs starting surface consists of 8 ML of InAs(001) grown on a GaSb buffer layer. (With a lattice mismatch of -0.6%, the InAs is well under the critical layer thickness and is therefore coherently strained.) As shown in Fig. 1(d), this surface consists of large terraces with very few islands or pits, similar to the GaSb(001) starting surface (terrace roughness="200 Å" roughness = 0 ML), but with terrace "fingers" elongated along the $[1\overline{10}]$ direction, and much more atomic-scale disorder. These two sources of roughness are evidence that the clean InAs surfaces are farther from equilibrium than the clean GaSb surfaces. Although the atomic-scale structure is not well ordered, the fingerlike shape of the terrace edges indicates that there is some reconstruction-related local order (consistent with RHEED): the [110]-oriented rowlike structure of As-terminated $InAs(001)2\times4$ promotes growth along this direction.¹³

The addition of an InSb layer to the strained InAs film further roughens the surface [Fig. 1(e)], with many large (300–500 Å), elongated islands appearing together with some generally smaller elongated pits (terrace roughness=2 ML). The terrace edges are also more jagged, which can be attributed to the growth mode whereby elongated islands are incorporated incompletely into the terrace edges. The asymmetric nature of the surface features is a further indication of a strong directional anisotropy in the growth of In on the InAs surface. Although this surface appears rougher than the InSb/GaSb one, the "200 Å" roughness is also approximately 1 ML due to the larger island size.

The roughest surface examined was the Sb-terminated GaAs interface on InAs [Fig. 1(f)], a surface with a very high density of interconnected islands. The islands are elongated in the [110] direction as in the InSb/InAs case, but with noticeably rounder edges. Note that many islands have become attached to the terrace edges, making it difficult to discern the underlying substrate terraces. However, based on the typical terrace width on the InAs surfaces, we estimate the roughness per terrace to be 3 ML (four layers are present, but the fourth layer is sparse). A 200 Å-long line along (100) would typically encompass three layers on this surface, corresponding to a roughness of 2 ML on this length scale.

Under our growth conditions, we find that the interfaces on GaSb surfaces are smoother than those on strained InAs, and that the InSb-like interfaces are generally smoother than GaAs-like ones on both surfaces ("200 Å" roughness of 1 ML versus 2 ML). These observations are consistent with the widths of identically grown interfaces measured with XHRTEM.⁷ Most significantly, the roughness we observe on the 200 Å length scale, associated with the island and pit shapes and size distributions, completely accounts for the interface widths observed via XHRTEM. Combined with previous x-ray diffraction data that demonstrate that the composition profiles of the epilayers are abrupt, and Raman spectra that show the expected bond types, ^{8,9} this result leads us to conclude that the roughness associated with growth is the primary source of disorder in our GaSb/InAs superlattice interfaces, with intermixing playing a minor, secondary role.

With the exception of the clean GaSb(001) surfaces, the surfaces examined do not appear to be near thermodynamic equilibrium. The types of roughness we observe on these interfaces (islands, pits, jagged terrace edges, etc.) are all indications of kinetically limited growth; i.e., at 400 °C the adatom and vacancy diffusion rates are too slow to keep up with the deposition rates. We attribute the relative roughness of the interfaces on InAs compared with those on GaSb in part to the rougher structure of the InAs starting surface. Another contribution may come from a difference in the relative mobilities of In and Ga on the InAs(001)2×4 versus $GaSb(001)1\times3$ surfaces: The multilayer island distribution on InAs suggests that the cations are less mobile on this surface. The cation mobilities may also play a role in the relative roughness of the InSb-like versus GaAs-like interfaces, given that a larger mobility of In versus Ga would result in comparatively smoother InSb-like interfaces. This effect will be enhanced by the lower deposition rate of In (0.2 ML/s) than Ga (0.5 ML/s). The relative cation mobilities are consistent with what one would expect based on the relative binding energies: GaAs>InAs>GaSb>InSb. 14

Although the interfaces examined here are under various degrees of strain due to the lattice mismatches with respect to GaSb (GaAs=-7.3%, InAs=-0.61%, InSb=+6.3%), there are no apparent correlations between the surface morphologies and strain. It is possible that the strain contributes to differences in the growth kinetics (and may ultimately prevent the creation of "perfect," atomically smooth interfaces), but we do not believe that the surfaces described here are composed of strain-related equilibrium structures.

An important issue related to MBE-grown interfaces is the role of the different anion surface coverages associated with the different surface reconstructions. For example, $GaSb(001)1\times3$ has an Sb coverage ~ 1.7 times that on a bulk-terminated 1×1 surface, ¹¹ but $InAs(001)2\times4$ has only $\sim 1/2$ the As coverage of the $1\times1.^{13}$ During MEE on GaSb the excess Sb may desorb or "float" on top, whereas on InAs there is no compensating source of anion, possibly contributing to the greater disorder observed on the InAs-based interfaces.

Review of the conditions used to grow the superlattices in which intermixing was found to be a significant source of interfacial disorder reveals a possible source of the discrepancies with our results. The interfaces in those superlattices were grown via codeposition following the interrupt, ^{5,6} as opposed to the MEE procedure used here (cation layer deposited by itself). We believe that codeposition allows anion exchange and diffusion at the interface so that, for example, an InAs epilayer grown on GaSb will have a multilayer interface composed of both InSb-like and GaAs-like bonds. This intermixing-related disorder will occur in addition to the type of roughness-related disorder we observe, resulting in more disordered interfaces. Moreover, the kinetics of the intermixing reactions are probably interface-dependent, which would further contribute to the different degrees of disorder observed on codeposited versus MEE-grown interfaces.

In summary, we have used STM to study the possible interfaces of MBE-grown short-period GaSb/InAs superlattices *in situ*. We conclude that the primary source of disorder at these interfaces is surface roughness associated with kinetically limited growth, and predict that significant reductions in interface roughness should be achievable by selectively tuning the MEE conditions (interrupts and flux rates) for each interface type. Smoother interfaces should result in enhanced electronic mobilities and, ultimately, better performing infrared detectors.

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